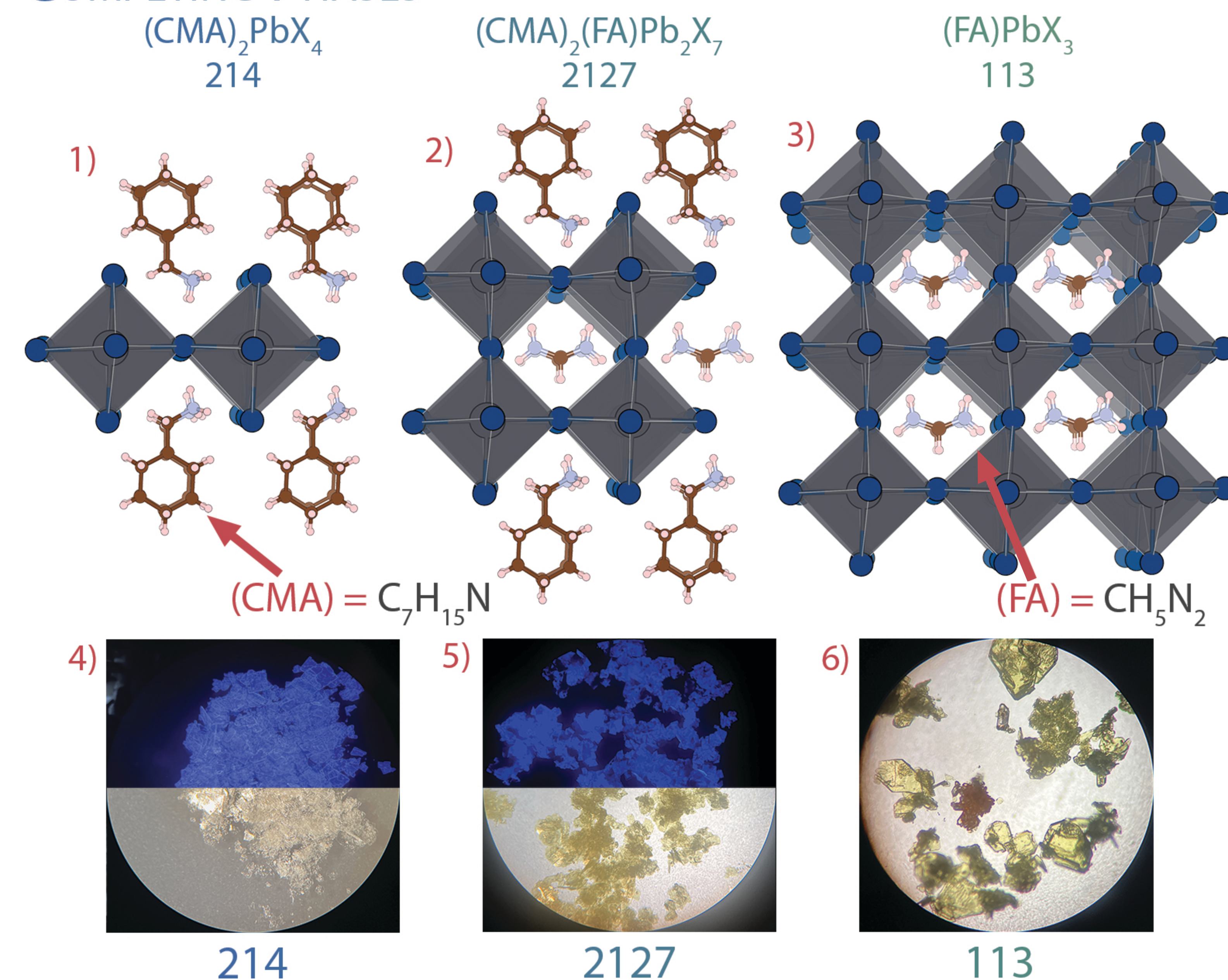


Synthesis of Novel Lead-Halide Perovskite $(\text{CMA})_2(\text{FA})\text{Pb}_2\text{Br}_7$ to Uncover Structure-Property Relationships

CONCEPTS & GOALS

- We synthesized the novel perovskite $(\text{CMA})_2(\text{FA})\text{Pb}_2\text{Br}_7$ to evaluate the structural descriptor χ ¹
- The structural descriptor is a quantity calculated from crystal structure parameters, correlated with PLQY
- This correlation was used to create $(\text{CMA})_2(\text{FA})\text{Pb}_2\text{I}_7$, which has the best PLQY for iodide materials
- Creating a bromide χ allows for the best bromide material to be predicted

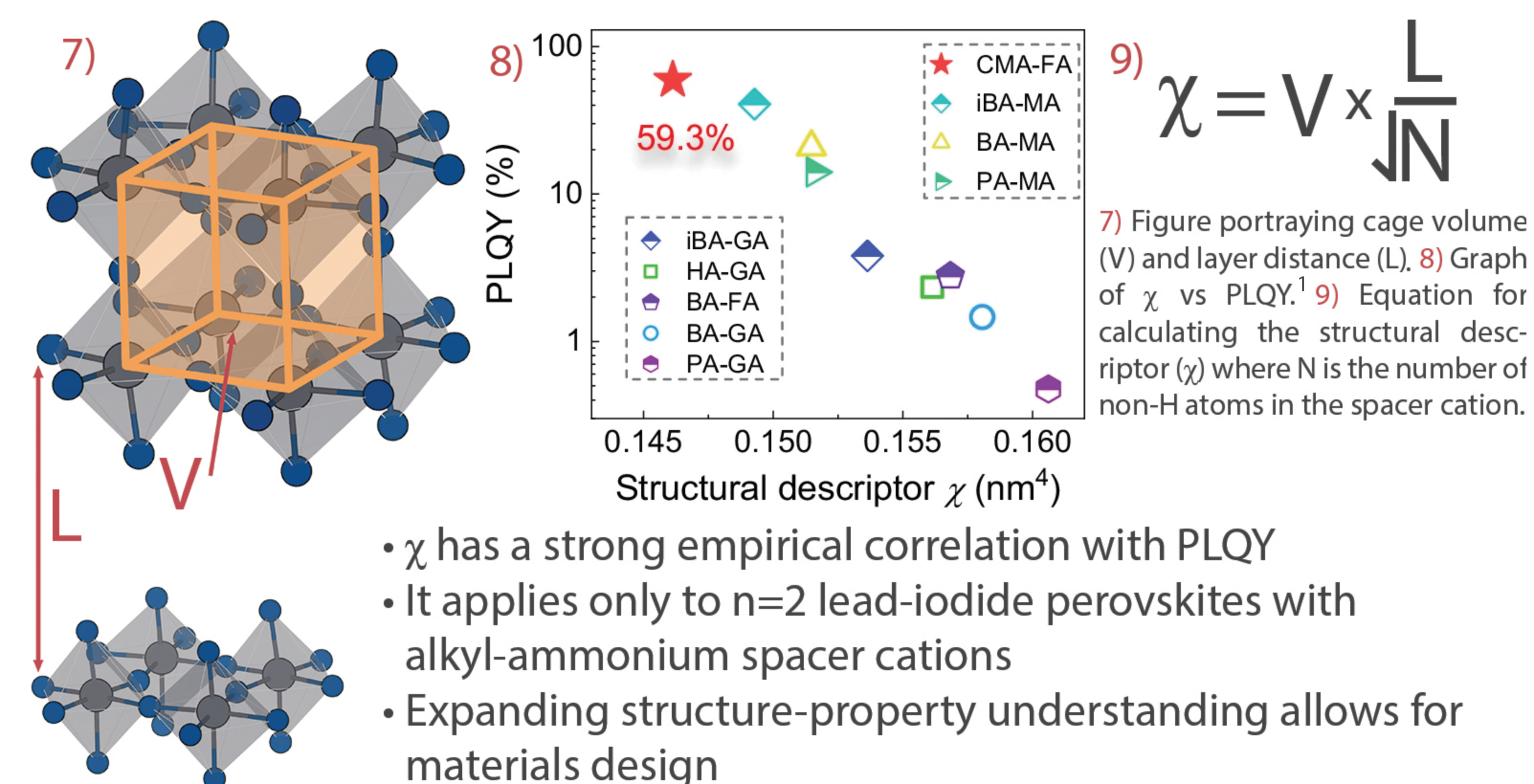
COMPETING PHASES



1-3) Example crystal structures for the different perovskite phases, 214 (1), 2127 (2), and 113 (3). 4-6) Images of the common impurity phases. 6) 113 forms as both orange crystals and yellow crystals that luminesce green.

- Current work is making a pure phase sample, we have synthesized $(\text{CMA})_2(\text{FA})\text{Pb}_2\text{Br}_7$
- Purity is difficult because 2127 shares precursors with 113 and 214.
- 214 and 113 impurities are constantly present, disabling our ability to measure PLQY

STRUCTURAL DESCRIPTOR

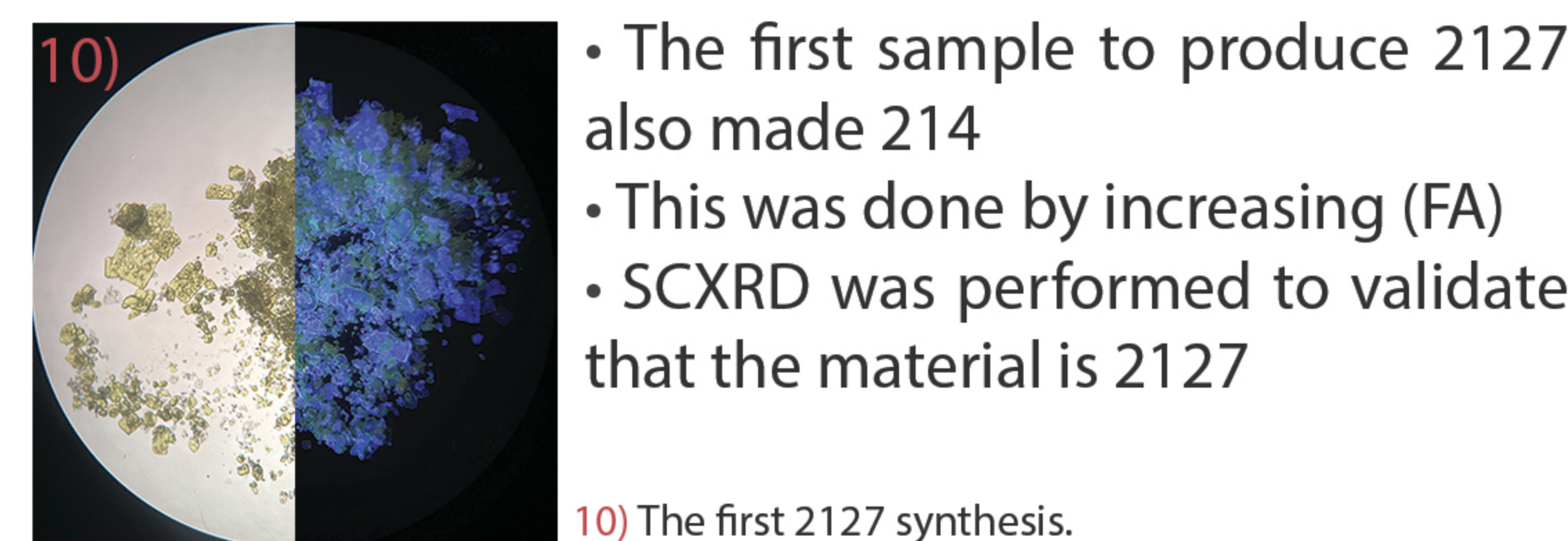


SYNTHESIS & IDENTIFICATION

Materials	(FA*HCl)	PbBr ₂	(CMA)	CH ₃ OH	HBr
Quantity	2 mmol	0.5 mmol	0.4 mmol	1.5 ml	5 ml

Procedure

- 1) Add (FA*HCl), PbBr₂, and (CMA) to HBr
- 2) Heat solution to 120°C
- 3) Add CH₃OH
- 4) Cool to room temperature
- 5) Vacuum to remove solution

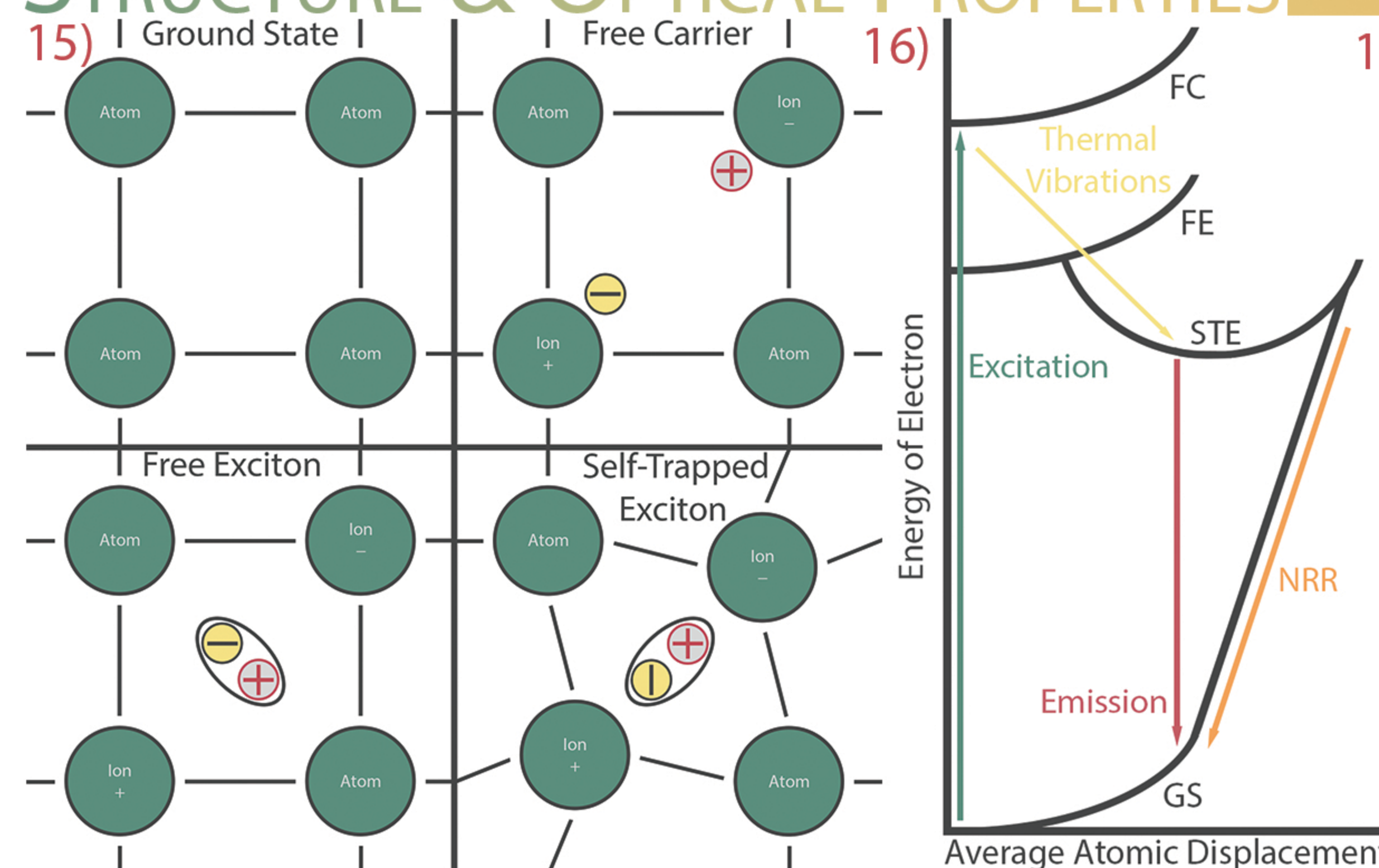


CONCLUSIONS

(CMA) and (FA) have hugely varied solubility within this solution
Phase formation is determined by the presence of these ions
When they are both present 2127 will form

My future work will involve adjusting the precursor quantities and solution make-up to present (CMA) and (FA) identically.

STRUCTURE & OPTICAL PROPERTIES



15) Graphic portraying how an excited electron can form bonds to lower its energy. 16) A graph symbolizing the energies of the electron states. NRR is non-radiative recombination.

- Lower-energy excitons define perovskite emission
- Free carriers cause reabsorption, STEs cause NRR
- Free excitons are correlated with the highest PLQY
- Structural Descriptor predicts exciton presence

FURTHER WORK

- Refine synthesis for purity by controlling the temperatures at which (CMA) and (FA) precipitate
- Collect PL and PLQY measurements on a pure sample
- Collect more bromide structural descriptor and symmetric factor data, establish correlation with iodide materials
- Synthesize all my work and author a paper

